Abstract

The present invention relates to a method and a system of identifying biologically active molecules. Evaluating receptor or target suitability of molecules is an important task in pharmaceutical drug research. With the increasing employment of automation techniques over the last years within Drug Discovery processes, methods like High-Throughput-Screening (HTS) and High-Throughput-Synthesis have become industry standards in pharmaceutical research. Nowadays, it is possible to test more than 20,000 molecules per day for their biological activities in certain disease targets. Also in the area of chemical synthesis, combinatorial chemistry in combination with automation processes, hundreds of molecules per day can be made physically available. Since based on today's chemical knowledge, more than 10^{100} molecules could theoretically be synthesized and tested and several hundreds of thousands molecules are commercially available, computer assisted methods have been developed to select subsets of molecules which are actually supposed to be tested based on their predicted potential of biological activity for certain disease targets.